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Counterflow diffusion flame of hydrogen-enriched biogas under MILD oxy-fuel condition

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ABSTRACT

Biogases are commonly found renewable fuels. Meanwhile they are difficult to be economically utilized because their low calorific values are very small and the induced costs of upgrading are expensive. To overcome the above deficiencies, in this paper we discuss the feasibility to utilize biogases under the MILD oxy-fuel operation recently proposed by the present authors. A popularly used counterflow configuration is adopted as the research prototype in this work. The effects of (1) the preheated temperature of the oxidizer mixtures, (2) the oxygen concentration in the oxidizer flow and (3) the hydrogen concentration in the fuel mixtures on the reaction structure of biogas under the new combustion condition are investigated with the aid of the lattice Boltzmann method (LBM). Through numerical simulation, it is found that the MILD oxy-fuel combustion fueled by biogas can be sustained even with relatively low preheated temperature of the oxidizer, extremely highly diluted oxygen concentration in the oxidizer flow and little hydrogen addition in the fuel mixtures, which provide a solid theoretical basis to develop a novel scheme to respond to the challenge caused by CO_2 emissions. Moreover, our discoveries imply the breakdown of the popularly used flamelet approach and emphasize the urgency to develop new turbulent combustion models for this novel combustion strategy.
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1. Introduction

According to the latest "World Energy Outlook" published by the International Energy Agency [1], CO_2 emitted by power plants will continue to constitute the major share of greenhouse gases in the next two decades due to the sharp increasing demand on electric power. However, the abrupt change in the Earth's climate system highlights the urgency to cut at least 50% of global greenhouse gases emissions from 2005 levels by 2050 [1]. The sharp increasing demand on electric power and the preservation of the global warming place the human being in a dilemma. In order to address this challenge, besides developing novel combustion technologies to reduce CO_2 emissions, it is desired to replace the conventional fossil fuels by renewable energy sources as far as possible. In order to curb greenhouse gases emissions to Copenhagen/Kyoto protocol compliant levels, combustion specialists have made significant efforts at least from three directions: (1) to replace conventional fossil fuels by renewable resources; (2) to retrofit/build power plants using conventional fossil fuels with the aid of novel combustion technologies; (3) to combine the former two ways organically.

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Among them, the last way is the most attractive one because it can accelerate the reduction of CO_2 emissions, although its complexity is the highest.

As Jahangirian et al. concluded in their work [2]: "Biogas", which typically originates from the anaerobic digestion of biomass and organic wastes by micro-organisms, is a renewable and biodegradable energy source that can be used for heating, lighting, transportation, small-scale power generation, and large gas turbines as a complementary fuel. The benefits of biogas are generally similar to those of natural gas. In addition, burning biogas reduces greenhouse gas emissions; it reduces the net CO_2 release and prevents CH_4 release. Thus, biogas combustion is a potential means to satisfy various legislative and ecological constraints." Up to date there have been numerous studies on the combustion characteristics of biogases. Henham and Makkar [3] discussed the combustion of biogases in a dual-fuel diesel engine over a wide range of compositions of gaseous mixtures. They focused on how to economically transform energy through biogases into the thermodynamically higher valued mechanical energy. Crookes [4] experimentally examined the emissions from spark- and compression-ignition engines using simulated biogas produced from domestic-supply natural gas. He observed that, for the simulated biogas which contained significant fractions of carbon dioxide, the emissions of oxides of nitrogen were reduced relative to natural gas, while unburnt hydrocarbons increased compared with natural gas or gasoline. The author systematically discussed the effects of adding increasing fractions of inert gases into the simulated biogas on the emissions of NO_x. Equivalent effects were also demonstrated with nitrogen replacing carbon dioxide in the simulated biogas. The influence of hydrogen addition on the performance of a biogas fueled spark ignition engine was investigated in Ref. [5]. It was observed that hydrogen significantly enhanced the combustion rate and extended the lean limit of combustion of biogases besides an improvement in brake thermal efficiency and brake power. The second-law based availability analysis in a spark ignition engine under biogas–hydrogen mixtures fueling conditions was conducted by Rakopoulos and Kyritsis [6] and Rakopoulos and Michos [7]. It was revealed that the addition of increasing amounts of hydrogen in biogases promoted the degree of reversibility of the burning process due to the incurred increase of combustion temperatures. Jahangirian et al.[2] investigated the thermal and chemical structures of biogases highly diluted by N_2 in counterflow diffusion flames. The authors found that, compared with pure methane, biogases could significantly reduce the net release of three greenhouse gases: CO_2, CH_4 and N_2O.

Among the recently emergent novel combustion technologies, the oxy-fuel [8] and MILD (moderate or intense low-oxygen dilution) [9] combustion technologies have attracted increasing attention. The oxy-fuel combustion is a process of burning fuel in a mixture of pure oxygen and recirculated flue gas [8]. Compared with convectional air-fired boilers, the exhaust gases in the oxy-fuel regime are composed mainly of CO_2 instead of N_2 since almost all atmospheric nitrogen has been removed from the input air, which makes it possible for Carbon Capture and Storage (CCS) with commercial requirements. The oxy-fuel technology was originally developed by the US Argonne National Laboratory. Within two decades, it has been developed from laboratory tests to industrial applications, which is an extraordinary progress as for an energy technology. However, the original oxy-fuel combustion strategy suffers from several shortcomings like flame instability and locally high temperature gradients [10]. The MILD combustion, usually being characterized by both an elevated temperature of reactants and low temperature increase in combustion processes, is judged as "one of the most promising combustion technologies in 21st Century" [9] due to its intrinsic advantages such as good combustion stability, enhanced heat transfer, high energy recovery and uniform distribution of chemical and thermodynamic variables. The publications on these two novel combustion technologies are nearly countless and the latest development of them can be found in some review papers [10–12]. Through high temperature recirculated flue gas, the oxy-fuel and MILD combustion technologies can be integrated seamlessly. The novel MILD oxy-fuel combustion strategy proposed by the present authors with the support from the US–China Clean Energy Research Center, is an improved variation of the original oxy-fuel combustion technology and can remedy its ancestor's deficiencies satisfactorily. The readers who are interested in this topic can refer to the review paper by the present authors [12].

Almost all existing publications on oxy-fuel and/or MILD combustion technologies are limited in discussing the performance of traditional fossil fuels under these novel combustion conditions. Up to date the corresponding literature on biogases in the new combustion regimes is still quite sparse. To the best knowledge of the present authors, until now there is only one publication [13] on this issue. In Ref. [13], the authors compared the performance of biogas and natural gas in the flameless combustion regime. Their results indicated that the flameless combustion regime eased the interchangeability between fuels of different compositions.

The above literature survey clearly shows that the investigation on the feasibility to utilize biogases under the MILD oxy-fuel condition is absent yet, whereas the potential benefits of this novel combination are obvious. It is well known that there are generally two drawbacks to utilize biogases in conventional modes: their low calorific values (LCVs) are too small and the induced costs of upgrading are very expensive. Upgrading means the removal of CO_2 from biogases to raise their LCVs. However, under the MILD oxy-fuel operation, these two disadvantages of biogases disappear naturally: the MILD combustion mode can work well even though the LCVs of used fuels are extremely small and in the oxy-fuel regime the removal of CO_2 from biogases is unnecessary because additional CO_2 is required to dilute the hot reactants. Although it is a promising way to utilize biogases more efficiently and economically, the necessary knowledge on this novel strategy is highly desired before it could be widely implemented with confidence in its performance.

The main originality of the present work is to investigate the reaction zone structure of biogas combustion in the MILD oxy-fuel regime for the first time. Hydrogen is added to sustain combustion. As a pioneering study, the influences of: (1) the preheated temperature of the oxidizer, (2) the oxygen concentration in the flow from the oxidizer side and (3) the hydrogen concentration in combustible mixtures in the fuel

side on the performance of biogas under the new combustion condition are investigated with the aid of numerical simulation. It is found that the MILD oxy-fuel combustion fueled by biogas can be sustained even with relatively low preheated temperature of the oxidizer, extremely highly diluted oxygen concentration in the oxidizer flow and little hydrogen addition in the fuel blends, which provide a solid theoretical basis to develop a novel scheme to respond to the challenge caused by CO_2 emissions. Moreover, our discoveries imply that the popularly used flamelet approach may breakdown under this novel combustion operation.

2. Specification of the problem and mathematical modeling

The opposed jet diffusion flame is a popular research prototype for the studies on MILD [14,15] and oxy-fuel [16,17] combustion technologies since a planar flame can be formed in the counterflow of reactants and the influences of lifted jet flame can be eliminated. Therefore a relatively simple while nontrival reaction zone structure can be obtained in such configuration. The configuration of planar opposing jets illustrated in previous studies conducted by the present authors [18–23] is adopted in this study again since such configuration is a typical one used in advanced combustion technologies research [25]. The problem domain and boundary conditions are summarized in Fig. 1. Two-dimensional rectangular coordinates are used and the origin of coordinates is located at the geometric center of the investigated domain. Two parallel stationary walls are located at $y = \pm L$ and the aspect ratio $A = L/W = 0.6$. The fuel mixture, which consists of hydrogen and biogas, is uniformly ejected from the bottom wall with temperature $T_{fuel} = T_0$ and the preheated oxygen diluted by CO_2 is uniformly ejected from the top wall with temperature T_{oxi}. The compositions of biogases vary based on the feedstock and in the present work the biogas is composed of 60% CO_2 and 40% CH_4 by volume ratio,

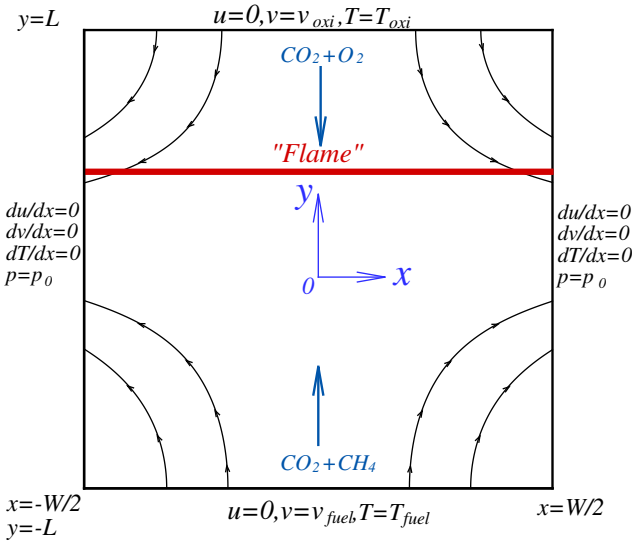


Fig. 1 – Schematic configuration and coordinate system of the computational domain.

namely the typical composition for biogas from active or recently closed landfills [2]. The counterflow impacts and reacts in the reaction zone. Then, a diffusion stagnation "flame" is formed and the burned gas flows outward along the x-direction.

The dimensionless governing equations in the Cartesian coordinates for such laminar reacting flows have been given in our previous studies [18–23] and a simple lattice Boltzmann (LB) model was proposed in them to solve the corresponding governing equations. During the last two decades or so, the LB method has matured as an efficient alternative and promising numerical scheme for simulating and modeling complicated physical and chemical systems [26,27]. Especially, it may be the best alternative of the traditional CFD technologies to deepen our insight into the MILD oxy-fuel combustion technology [28]. Until now it has been widely accepted that, compared with conventional combustion scenarios, the molecular diffusion will play an important role in the MILD [29] and/or oxy-fuel [10] regimes. However, the traditional CFD technologies cannot meet the challenges because the micro-scale molecular diffusion is often mis-represented within the frameworks of conventional CFD, especially in low numerical-resolution computation. On the contrary, the LB method can accurately represent microscopic physics such as molecular diffusion and chemical reactions due to its kinetic nature [28]. Moreover, the assumption of scale separation, which is the basis for "continuum" CFD to build turbulent models, is not required in the LB method any longer [30].

In the present study, $v_{fuel} = v_0 = 0.1$ is the mean dimensionless inlet velocity of the fuel flow. $p_0 = 1/3$ and $T_0 = 1$ (corresponding to 300 K) are the dimensionless reference pressure and temperature, respectively. The dimensionless characteristic length $L = 1$. The inlet Reynolds number of the oxidizer flow is defined as [20]:

$$Re_{oxi} = \frac{v_{oxi} L}{\upsilon_{oxi}}, \tag{1}$$

where υ_{oxi} is the kinematic viscosity of the oxidizer mixture. The inlet Reynolds number of the fuel flow is determined by

$$Re_{fuel} = \frac{v_{fuel} L}{\upsilon_{fuel}}. \tag{2}$$

where υ_{fuel} is the kinematic viscosity of the fuel mixture. The thermodynamic and transport properties appearing in the governing equations are given in [31]. In the present study, Re_{fuel} is fixed and Re_{oxi} will vary according to the concentration of oxygen in the oxidizer flow and that of CH_4 and H_2 in the fuel flow so to guarantee the effective equivalence ratio [23] as unity. Consequently the strain rate [21–23] in the counterflow will change accordingly. The reason why we keep a fixed effective equivalence ratio instead of a fixed strain rate is that the emphasis of the present study is to reveal the feasibility of utilizing biogas under the MILD oxy-fuel operation instead of the fine reaction structure of biogas in this new regime. What should be mentioned is that in the present study all quantities used in the LB computation are dimensionless. The detailed normalized process can be found in [18–23,27].

As a preparatory study, in this work we just focus on the effects of: (1) the preheated temperature of the oxidizer, (2) the oxygen concentration in the flow from the oxidizer side and

(3) the hydrogen concentration in the fuel blends on the performance of biogas under the MILD oxy-fuel operation, so the global chemical reaction mechanisms recently proposed by the present authors [32] for hydrogen-enriched biogas combustion under the novel condition are adopted:

$$CH_4 + 1.5O_2 \rightarrow CO + 2H_2O, \tag{3}$$

$$CO + 0.5O_2 \rightleftharpoons CO_2, \tag{4}$$

$$H_2 + 0.5O_2 \rightleftharpoons H_2O, \tag{5}$$

$$\omega_{ov} = k_{ov} T^{\beta} \prod_{j=1}^{N} \left(\frac{\rho Y_j}{W_j}\right)^{\alpha_j} \exp(-E/RT), \tag{6}$$

where β is the temperature exponent; ω_{ov} is the overall reaction rate; k_{ov} is the reaction coefficient; E is the effective activation energy; R is the universal gas constant and α_j, Y_j and W_j are the reaction exponent, mass fraction and molecular weight of the jth reactant, respectively. The corresponding reaction rate data in the above global chemical reactions are given in Table 1. The rate constants in this table are collected from [33,34].

The volume percentage of hydrogen in the fuel blends X_h is defined as [18,22]

$$X_h = \frac{V_h}{V_h + V_b}, \tag{7}$$

where V_h and V_b are the volume fractions of hydrogen and biogas in the mixtures, respectively. Similarly, for the oxidizer mixtures there is

$$X_o = \frac{V_o}{V_o + V_c}, \tag{8}$$

where V_o and V_c are the volume fractions of oxygen and carbon dioxide in the mixtures, respectively.

3. Solution procedure

The LB model proposed in our previous studies [19,20] is used to solve the governing equations for the reacting flow, namely to solve the flow field by

$$g_k(\vec{x} + c\vec{e}_k \Delta t, t + \Delta t) - g_k(\vec{x}, t) = -\tau_u^{-1}\left[g_k(\vec{x}, t) = g_k^{(eq)}(\vec{x}, t)\right], \tag{9}$$

and to solve the temperature T and mass fractions Y_i ($i = O_2$, H_2, CH_4, CO_2, CO, H_2O) by

$$f_{\psi,k}(\vec{x} + c\vec{e}_k \Delta t, t + \Delta t) - f_{\psi,k}(\vec{x}, t) = -\tau_{\psi}^{-1}\left[f_{\psi,k}(\vec{x}, t) - f_{\psi,k}^{(eq)}(\vec{x}, t)\right] + \zeta_k Q_{\psi} \Delta t, \tag{10}$$

In the above equations the subscript k means the discrete velocity directions and $\Psi = Y_i, T$ respectively. In this study, the D2Q9 lattice model [35] is used, i.e. $k = 9$. In Eqs. (9) and (10) g_k and f_k are the distribution functions for the flow, temperature and concentration fields. The superscript eq represents the corresponding equilibrium parts. τ_u, τ_Ψ, $\vec{e}_k$, ζ_k and Δt are the relaxation times, discrete velocities, weight coefficients and time step of the LB model, respectively. Q_Ψ is the source term due to chemical reactions [19,20]. The full spectrum k-distribution approach proposed by Modest et al. [36] is employed to model the radiation heat transfer and the LB scheme designed by Mishra et al. [37] is adopted to include the radiation heat flux into the evolution equation Eq. (10) for the temperature field. The flow velocity, temperature and mixture fraction of species i are obtained by

$$\vec{u} = \frac{1}{\rho} \sum_k c\vec{e}_k g_k, \tag{11}$$

$$\Psi = \sum_k f_{\psi,k}, \quad (\Psi = Y_i, T), \tag{12}$$

Because the distribution functions at the boundaries are unknown, the non-equilibrium extrapolation scheme used in our previous studies [19,20] is employed to treat the flow, temperature and concentration boundary conditions, namely

$$g_k|_w = g_k^{eq}|_w + g_k^{non-eq}|_w = g_k^{eq}|_w + \left(g_k|_f - g_k^{eq}|_f + O(\in^2)\right), \quad g_k|_w = g, \tag{13}$$

$$f_{\psi,k}|_w = f_{\psi,k}^{eq}|_w + f_{\psi,k}^{non-eq}|_w = f_{\psi,k}^{eq}|_w + \left(f_{\psi,k}|f - f_{\psi,k}^{eq}|_f + O(\varepsilon^2)\right), \tag{14}$$

where the subscript w and f represent the wall boundary grid and the nearst-neighbouring fluid grid respectively. ε is a small quantity [22]. The computer program will terminate when the reactive flow becomes steady. The detailed description can be found in our previous publications [20,22].

4. Numerical validation

The validation consists of two parts: the validation of the global chemical reaction mechanisms used in the present

Table 1 – Global combustion mechanisms with kinetic rate data from [33,34] (units in kmol, m^3, K, s, KJ).

Reaction mechanism		Rate orders	β	k_{ov}	E/R
$CH_4 + 1.5O_2 \rightarrow CO + 2H_2O$	(R1)	$[CH_4]^{0.7}[O_2]^{0.8}$	0	5.03×10^{11}	24,056
$CO + 0.5O_2 \rightarrow CO_2$	(R2)	$[CO][H_2O]^{0.5}[O_2]^{0.25}$	0	2.24×10^{8}	5032
$CO_2 \rightarrow CO + 0.5O_2$	(R3)	$[CO_2][H_2O]^{0.5}[O_2]^{-0.25}$	−0.97	1.10×10^{13}	39,452
$H_2 + 05O_2 \rightarrow H_2O$	(R4)	$[H_2][O_2]^{0.5}$	0	7.91×10^{10}	17,609
$H_2O \rightarrow H_2 + 0.5O_2$	(R5)	$[H_2O]$	0	3.48×10^{13}	47,907

study and the validation of the LB code for the adopted counterflow combustion research prototype.

To validate the global chemical reaction mechanisms listed in Table 1, firstly the JHC burner proposed by Dally et al. [38] is simulated with the aid of the finite volume method (FVM) based commercial software Fluent 6.1.22. Fig. 2 illustrates the numerical results obtained by the present global chemical reaction mechanisms together with the experimental data published in [38]. The validity of the global chemical reaction mechanisms listed in Table 1 can be demonstrated by the good agreement between numerical and experimental data.

In order to validate the performance of the LB approach under the MILD oxy-fuel condition, then we simulate the counterflow diffusion combustion with $Re_{fuel} = 200$, $X_h = 0.5$, $T_{oxi} = 5T_0$ and $X_o = 0.03$. The grid resolution 300×180 is used in this work for the LB computation. It has been demonstrated in our previous studies [18–23] that such grid resolution is fine enough to obtain grid-independent numerical solutions for the reactive flow investigated in this study. Fig. 3 illustrates the distributions of temperature and CO mass fraction along the line $x = 0$ obtained by the present LB approach together with that obtained by Fluent 6.1.22 with GRI-Mech 3.0. The numerical results obtained by these two methods agree very well. The slight discrepancies between the LBM and FVM solutions may be result from the different reaction mechanisms adopted in them.

In general, the flame thickness obtained by a reduced chemical reaction mechanism may be much broader in comparison to those adopting detailed reaction mechanisms. However, through Figs. 2 and 3, we observe that, at least for the major species, the influences of different reaction mechanisms on the cases investigated in the present work are not significant. Yet it is important to bear in mind on the possible discrepancies caused by reduced mechanisms.

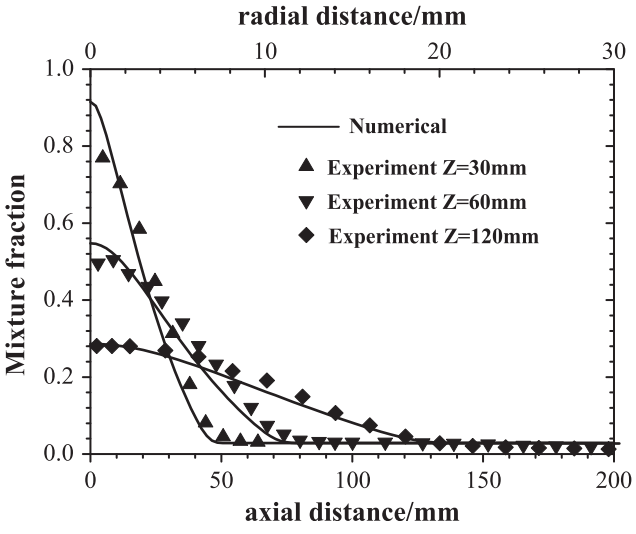


Fig. 2 – Comparison of mixture fraction profiles between numerical and experimental data along the axis and the radii of the JHC burner at Z = 30 mm, Z = 60 mm and Z = 120 mm.

5. Results and discussions

To investigate the influences of: (1) the preheated temperature of the oxidizer, (2) the oxygen concentration in the flow from the oxidizer side and (3) the hydrogen concentration in the fuel blends on the performance of biogas under the MILD oxy-fuel condition, in this study the Reynolds number and inlet temperature of the fuel mixtures are fixed at $Re_{fuel} = 200$ and $T_{fuel} = T_0 = 1.0$ while the rest parameters vary as $0 \le X_h \le 0.5$, $0.03 \le X_o \le 0.09$ and $3T_0 \le T_{fuel} \le 5T_0$. The behaviors of the various results are considered by assuming one of these parameters varying while the others are constant values.

5.1. *Effect of hydrogen addition in fuel blends*

The cases with $0 \le X_h \le 0.5$ at $T_{oxi} = 5T_0$ and $X_o = 0.03$ are chosen as the representatives to reveal the effect of hydrogen addition in the fuel blends.

Fig. 4 illustrates the profiles of temperature along the line $x = 0$ with various X_h. Through this figure, an obvious temperature peak due to the exothermic reactions can be observed when $X_h > 0.05$. The temperature peak reduces with the decrease of X_h. While $X_h < 0.05$, such temperature peak cannot be seen although the moderate chemical reactions are

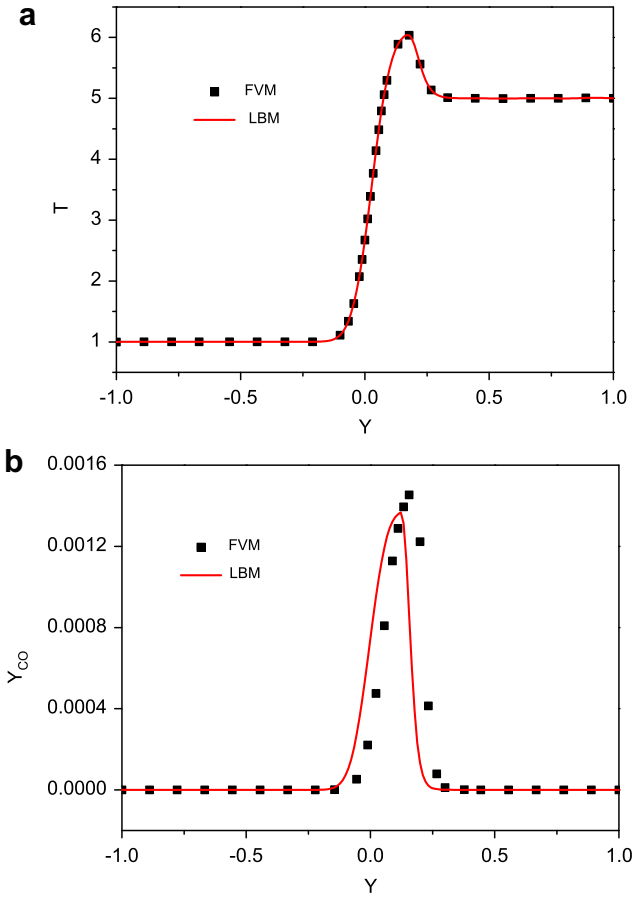


Fig. 3 – Distributions of (a) temperature (b) mass fraction of CO along line $x = 0$ at $Re_{fuel} = 200$, $X_h = 0.5$, $T_{oxi} = 5T_0$ and $X_o = 0.03$.

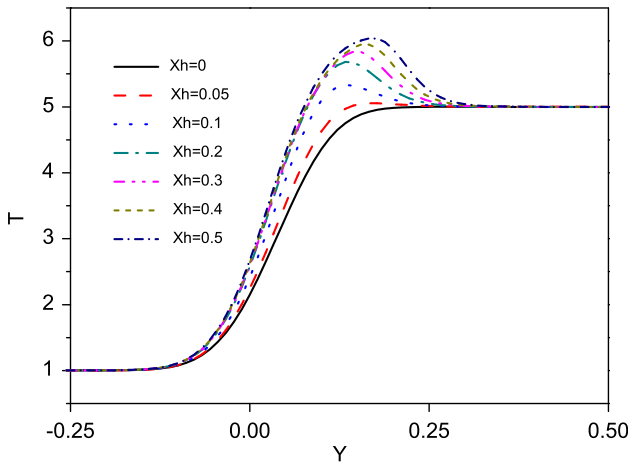


Fig. 4 – Distributions of temperature of various X_h along line $x = 0$ at $T_{oxi} = 5T_0$, $T_{fuel} = T_0$ and $X_o = 0.03$.

still going on under those conditions, as shown in Fig. 5. According to the same figure, one can observe that the reaction (R1) in Table 1 is the slowest step within the exothermic reaction chain, so it becomes the control step in the rate-limiting processes under the MILD oxy-fuel operation.

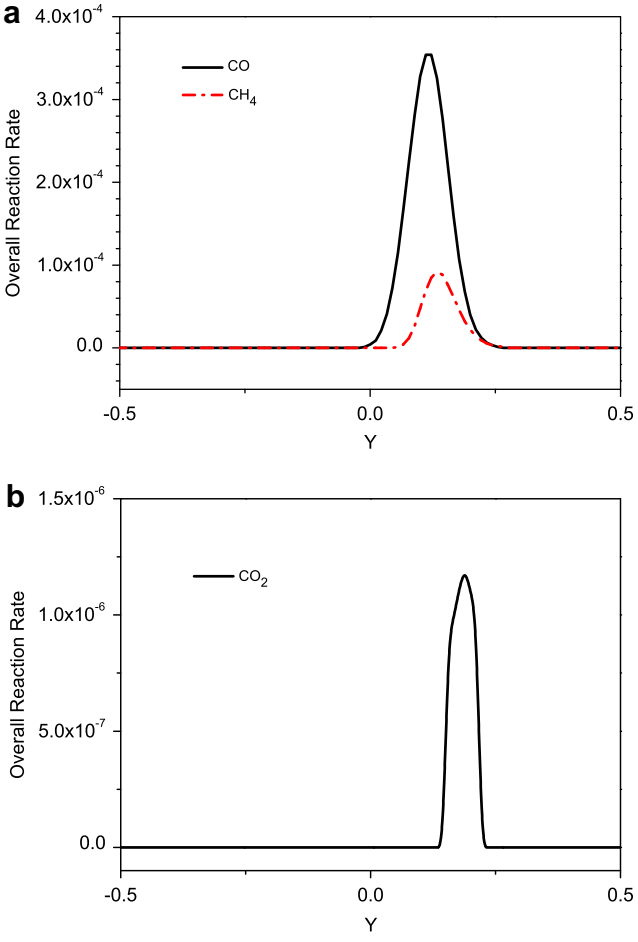


Fig. 5 – Overall reaction rates of (a) CH_4 and CO (b) CO_2 along line $x = 0$ at $X_h = 0$, $T_{oxi} = 5T_0$ and $X_o = 0.03$.

The variation of the maximum temperature T_{max} in the reactive flow versus X_h is plotted in Fig. 6. As shown in this figure, T_{max} increases with more hydrogen being added into the fuel blends since the calorific value of hydrogen is much higher than that of biogas used in this work. When $X_h < 0.05$, the increment of T_{max} is relatively small while significant as $X_h > 0.05$. This observation is consistent with that in Fig. 4. However, the increasing speed of T_{max} will decrease against X_h. There is an approximately power-function-like relationship between T_{max} and X_h, which reads $T_{max} = 6.39582X_h^{0.07791}$ as $X_h > 0.05$. The reduction of increasing speed of T_{max} mainly results from two mechanisms: Firstly, the volume of reaction zone with higher temperature will increase with more H_2 being added (see Fig. 4). However, it is well known that the radiative heat loss is proportional to the volume of reaction zone with higher temperature, which will reduce the peak temperature of "flame" [17]. Secondly, the endothermic reactions (i.e. Reactions (R3) and (R5) listed in Table 1) will be enhanced due to the increase of flow temperature, which also will reduce the peak temperature of "flame". Especially, owing to the extremely high concentration of CO_2 in the blends under the oxy-fuel condition, the contribution of Reaction (R3) to thermal patterns becomes significant, as illustrated in Fig. 7. According to this figure, one can see when the temperature in the reaction zone is high enough due to the addition of hydrogen, the overall reaction rate of the endothermic reaction (i.e. Reaction (R3)) will be comparable with that of its exothermic counterpart (i.e. Reaction (R2) in Table 1). However, if the temperature in the reaction zone is relatively low, compared with its exothermic counterpart (R2), the overall reaction rate of the endothermic reaction (R3) is extremely low (cf. Fig. 5). Consequently, the influence of the endothermic reactions on reduction of peak temperature can be neglected when X_h is very small.

The distributions of mass fractions of CH_4, H_2 and O_2 at two X_h are presented in Fig. 8. Even X_h up to 0.5, the investigated combustion cases in this subsection are still in the MILD regime, so the reaction zone structures with different X_h all are very similar to the so-called Liñán' premixed flame regime [14] despite a diffusion combustion configuration being

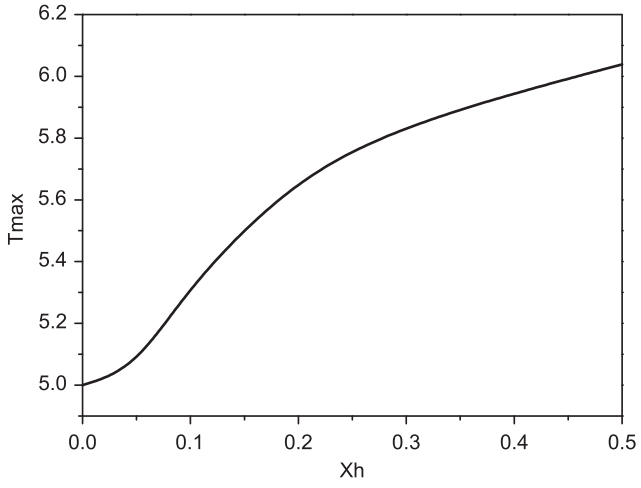


Fig. 6 – The maximum temperature versus X_h at $T_{oxi} = 5T_0$, $T_{fuel} = T_0$ and $X_o = 0.03$.

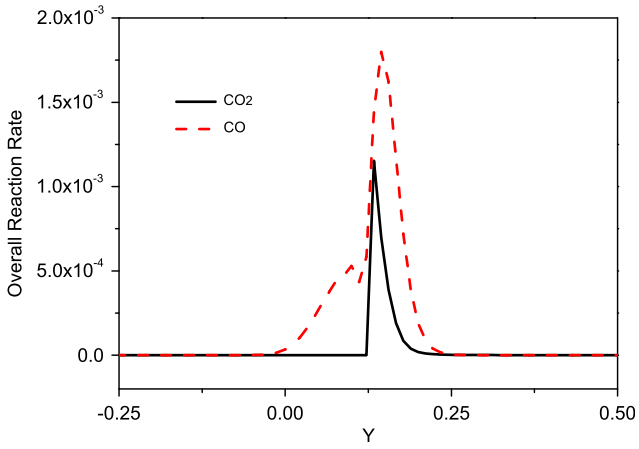


Fig. 7 – Overall reaction rate of CO and CO_2 along line $x = 0$ at $X_h = 0.5$, $T_{oxi} = 5T_0$ and $X_o = 0.03$.

adopted in the present study: O_2, H_2 and CH_4 concentration distributions cross over, which implies that the fuels and oxidizers are not consumed at a thin "'flame" region. It is quite different from their conventional air combustion counterpart [22,23] and perhaps is an intrinsic feature of the MILD combustion [14].

According to the above discussion, one can conclude: even for extremely low-oxygen concentration (e.g. $X_o = 0.03$ in the oxidizer flow), there is no necessity to add much hydrogen into the fuel blends to sustain the MILD oxy-fuel combustion using small LCV biogas which mostly consists of CO_2. This discovery supports the commercial possibility to utilize biogas under the MILD oxy-fuel condition in practical applications due to the high cost of producing hydrogen.

5.2. *Effect of oxygen concentration in oxidizer flow*

In this subsection, the cases with $0.03 \le X_o \le 0.09$ at $T_{oxi} = 5T_0$ and $X_h = 0$ are chosen as the typical ones to demonstrate the influences of oxygen concentration in the oxidizer flow on the reaction zone structure.

Fig. 9 illustrates the profiles of temperature along the line $x = 0$ with various X_o. As shown in this figure, when $X_o > 0.07$ an obvious temperature peak due to the exothermic reactions appears. When $X_o > 0.08$, the temperature peak increases quickly and the MILD regime will breakdown if X_o becomes big enough (e.g. $X_o > 0.085$). As $X_o > 0.085$ the temperature profiles are similar to that under high temperature air combustion (HiTAC) conditions [22,23]. HiTAC typically indicates to preheat air temperature by recycled heat from exhaust gases so high (approximately 1000 K) that the extinction curves of reactants disappear [24]. It can be observed more clearly through Fig. 10, where the variation of the maximum temperature T_{max} of the reactive flow versus X_o is plotted: firstly the slope of the curve is quite slight but becomes steep when $X_o > 0.08$, which denotes T_{max} is insensitive to X_o if the value of X_o is small enough.

Fig. 11 plots the distributions of mass fractions of CH_4 and O_2 at $X_o = 0.03$ and $X_o = 0.09$. According to this figure, we find that the thin flamelet assumption [25] popularly used in turbulent combustion simulations stands only when the concentration of oxygen is high enough (e.g. $X_o = 0.09$), that is, CH_4 and O_2 are consumed at a thin flame region and their reaction rates can be regarded as sufficiently high (see Fig. 12).

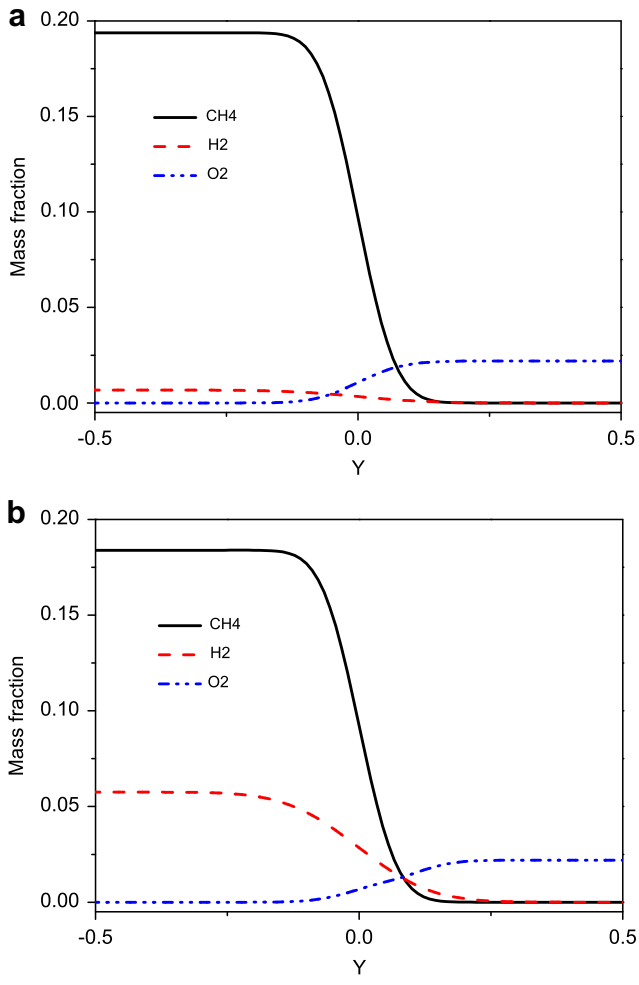


Fig. 8 – Distributions of mass fraction of CH_4, H_2 and O_2 with (a) $X_h = 0.1$ (b) $X_h = 0.5$ at $T_{oxi} = 5T_0$ and $X_o = 0.03$.

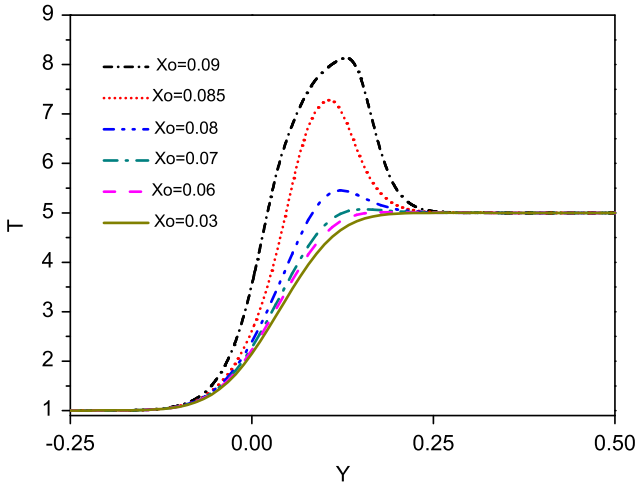


Fig. 9 – Distributions of temperature of various X_o along line $x = 0$ at $T_{oxi} = 5T_0$, $T_{fuel} = T_0$ and $X_h = 0$.

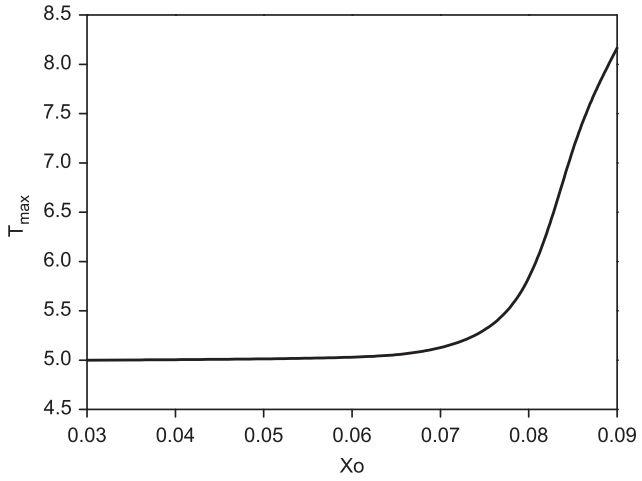


Fig. 10 – The maximum temperature versus X_o at $T_{oxi} = 5T_0$, $T_{fuel} = T_0$ and $X_h = 0$.

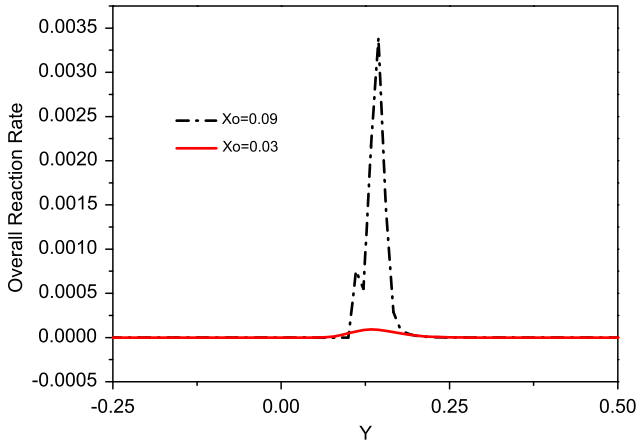


Fig. 12 – Overall reaction rate of CH_4 with various X_o at $T_{oxi} = 5T_0$ and $X_h = 0$.

While in the MILD regime, compared with its conventional air combustion counterpart, the fuels and oxidizers can coexist within a much wider zone and accordingly the validity of the flamelet assumption is questionable. Through Fig. 12, one can observe that the peak value of reaction rate of CH_4 at $X_o = 0.09$ is two orders of magnitude higher than that at $X_o = 0.03$ but the reaction zone in the latter is obviously wider than that in the former. The purpose to emphasize the flamelet assumption may be invalid in the MILD regime is induced by that recently there emerges the trend to invoke flamelet models to investigate the MILD combustion either in the Large-eddy simulations (LES) framework [39] or by the Reynolds-averaged Navier–Stokes (RANS) formulations [40]. In the combustion science community it has been aware that an adequate approach to describe turbulent non-premixed flames undergoing significant departures from chemical equilibrium through super-equilibrium radical concentrations and some aspects of pollutant formation is lacking yet [28,41]. The flamelet approach may be a promising tool to meet this challenge in a conventional air combustion mode but not in the MILD regime from the theoretical viewpoint because a flamelet model works well only when two assumptions that (1) the chemical time-scale is much faster than the fluid mixing time-scale and (2) the differential diffusion in the mixtures can be neglected both can hold [25]. Unfortunately, in the MILD regime neither of these two assumptions can be met [12,29]. Thus it is still an urgent task to develop suitable models to deepen our insight into this field. As concluded in the latest book on turbulent combustion modeling [41], although the available state-of-the-art CFD technologies have achieved great successes in combustion research concerned primarily phenomena in which the separation of scales can be justified, their applicability is seriously challenged by combustion in the regimes where both chemistry and mixing are competitive and/or turbulence-combustion interactions become more complicated due to overlapping time and length scales. However, as mentioned above, the MILD oxy-fuel combustion is characterized by these regimes, so the popularly used "continuum" CFD tools based on macroscopic models have great difficulties to meet these challenges. While as mentioned in Section 2, the LB approach, which is based on microscopic models and mesoscopic kinetic equations, may be the most promising candidate to achieve this goal. The potential of the LB method as a promising tool to advance combustion research also has been highlighted in [41].

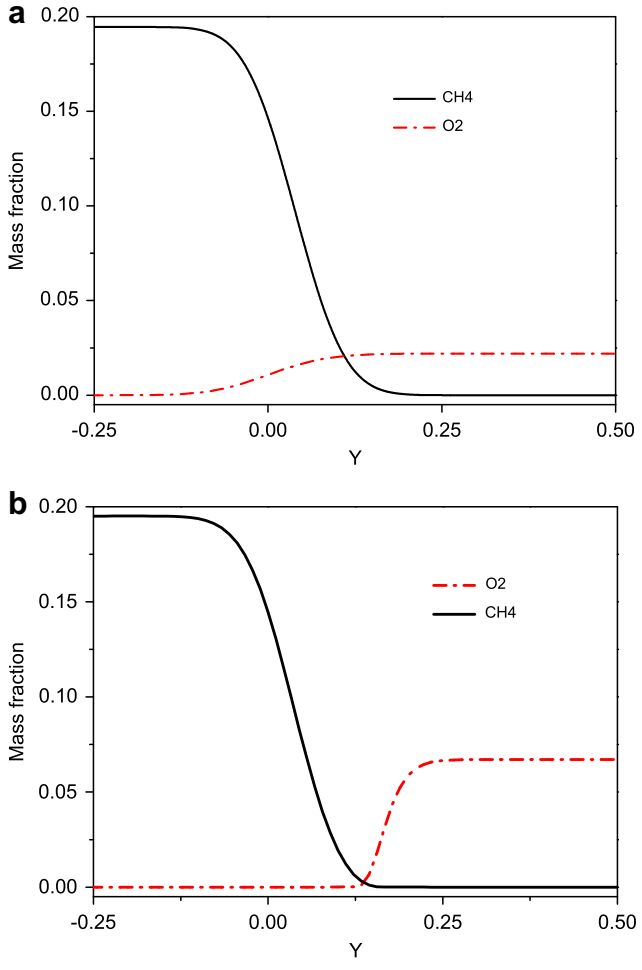


Fig. 11 – Distributions of mass fraction of CH_4 and O_2 with (a) $X_o = 0.03$ (b) $X_o = 0.09$ at $T_{oxi} = 5T_0$ and $X_h = 0$.

Through the above analysis, we can conclude that lower oxygen concentration in the oxidizer flow is better than higher one to form the MILD oxy-fuel combustion of biogas investigated in the present study. It is a good news for utilizing biogas in the MILD oxy-fuel regime since it is expensive to separate pure oxygen from air [10].

5.3. *Effect of preheated temperature of oxidizer flow*

As concluded in previous studies [9,12], the preheated temperature of oxidizer flow plays a very important role to form the MILD combustion. Through numerical simulations, we find that there will be no reaction if the preheated temperature of the oxidizer flow T_{oxi} is less than $4T_0$ (corresponding to 1200 K) and the influences of hydrogen addition in the fuel blends and the oxygen concentration in the oxidizer flow on the reaction zone structure, temperature, etc. all depend closely on T_{oxi}.

Fig. 13 plots the distributions of temperature of different X_h at $T_{oxi} = 4T_0$ and $T_{oxi} = 5T_0$. For the cases with $T_{oxi} = 4T_0$, the profiles of temperature at $X_h = 0$ and $X_h = 0.1$ are nearly the same. Namely at this level of preheated temperature the reaction zone structure is insensitive to hydrogen addition. However, with a higher preheated temperature of oxidizer

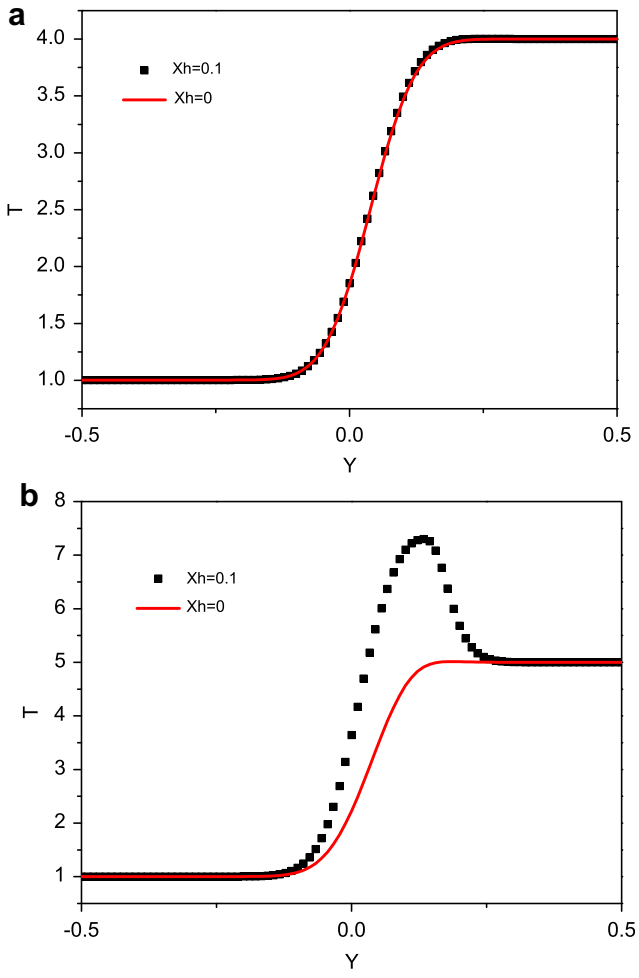


Fig. 13 – Distributions of temperature of various X_h with (a) $T_{oxi} = 4T_0$ and (b) $T_{oxi} = 5T_0$ along line $x = 0$ at $T_{fuel} = T_0$ and $X_o = 0.06$.

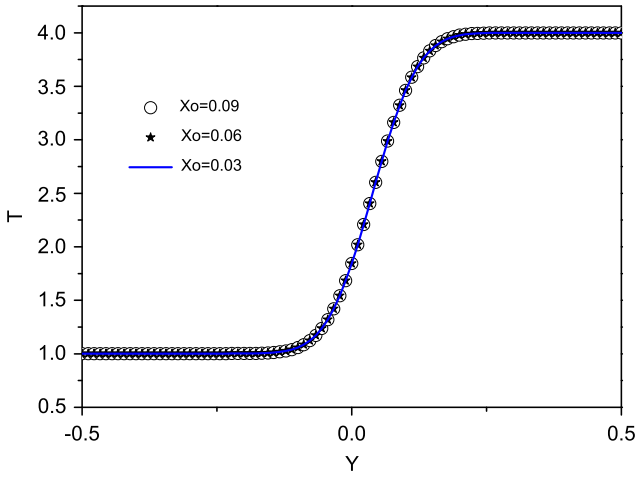


Fig. 14 – Distributions of temperature of various X_o along line $x = 0$ at $T_{oxi} = 4T_0$, $T_{fuel} = T_0$ and $X_h = 0$.

flow (e.g. $T_{oxi} = 5T_0$), the distributions of temperature at $X_h = 0$ and $X_h = 0.1$ are quite different even though the added hydrogen is relatively small, and there appears a significant temperature jump when $X_h = 0.1$, which denotes the MILD regime has broken down.

The profiles of temperature of various X_o at $T_{oxi} = 4T_0$ are illustrated in Fig. 14. With a relatively low preheated temperature, these three curves almost overlap each other. Namely at $T_{oxi} = 4T_0$ the reaction structure is insensitive to X_o. While as mentioned above, when $T_{oxi} = 5T_0$ the temperature distributions depend sensitively on X_o, especially when X_o is big enough (cf. Fig. 9).

Based on the above comparison, the crucial role of T_{oxi} on the MILD oxy-fuel combustion is obvious. In previous literature [14] it was claimed that the flameless combustion in methane–air counterflow can be sustained only when $T_{oxi} \geq 1500$ K, so under oxy-fuel conditions, the MILD combustion is more easily sustained than its air combustion counterpart, agreeing with our previous conclusion [12]. Especially, one of the present authors observed similar phenomena for a co-flow-jet configuration [42]. In [42], the authors found that for a JHC burner, the MILD regime can be organized more easily under the oxy-fuel condition than its air counterpart. Moreover, according to the aforementioned discussion, it can be concluded that lower T_{oxi} is safer to sustain the MILD regime for hydrogen-enriched biogas combustion under fluctuant input/operation.

6. Conclusion

In order to address the global warming challenge, it is desired to develop new combustion technologies and adopt renewable fuels as their chemical feedstock. The MILD oxy-fuel combustion strategy proposed by the present authors is a promising technology to reduce CO_2 emissions and we find that biogas, a commonly found renewable energy source with small LCV, may be utilized more efficiently and economically in this way. In order to demonstrate the feasibility, in this study the influences of [1] the preheated temperature of the

oxidizer, [2] the oxygen concentration in the flow from the oxidizer side and [3] the hydrogen concentration in the fuel blends on the performance of biogas under the new combustion condition are investigated with the aid of numerical simulation. The observations are quite positive:

1. Even for extremely low-oxygen concentration in the oxidizer flow, there is no necessity to add much hydrogen to sustain the MILD oxy-fuel combustion of biogas which mostly consists of CO_2;
2. Lower oxygen concentration in the oxidizer flow is better than higher one to form the MILD oxy-fuel combustion of biogas from landfills;
3. Compared with the air atmosphere, the MILD combustion is more easily sustained under oxy-fuel conditions. Especially, a lower preheated temperature is safer than a higher one to sustain the MILD regime for hydrogen-enriched biogas combustion under fluctuant input/operation.

These discoveries all imply that the utilization of biogas under the MILD oxy-fuel combustion operation up to commercial-scale is feasible and its implementation will significantly reduce the high costs induced by the currently utilizing way because the expensive step-"upgrading" can be avoided.

Besides above conclusions, we also confirm that the flamelet assumption breaks down in the MILD oxy-fuel regime. Because the available models cannot describe such reactive flow satisfactorily [28], it is expected to develop new turbulent combustion models to describe combustion under the new operation. It is promising to achieve this goal within the LB framework and it is the objective in our future work.

Acknowledgments

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